Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 364 °C

Global applicability domain: Inside

Local applicability domain index: 3.31e-01

Confidence level: 7.66e-01

Nearest Neighbors from the Training Set

Image not found

Tribenzylamine
Measured: 385
Predicted: 366

Image not found

Oxyfluorfen
Measured: 358
Predicted: 353

Image not found

Triphenylamine
Measured: 365
Predicted: 347

Image not found

Oxazole, 2,5-diphenyl-
Measured: 360
Predicted: 343